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data_iss2

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_chemical_formula_moiety          ?
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 'C62.33 H138 N4 O37 Si4 W9'
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 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0492   0.0322
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Si'  'Si'   0.2541   0.3302
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'W'  'W'  -5.4734   5.5774
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0311   0.0180
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_symmetry_space_group_name_H-M    'R 3 c'

loop_
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 '-y, x-y, z'
 '-x+y, -x, z'
 '-x+y, y, z+1/2'
 'x, x-y, z+1/2'
 '-y, -x, z+1/2'
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 '-y+2/3, x-y+1/3, z+1/3'
 '-x+y+2/3, -x+1/3, z+1/3'
 '-x+y+2/3, y+1/3, z+5/6'
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_diffrn_reflns_limit_k_min        -24
_diffrn_reflns_limit_k_max        24
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_computing_cell_refinement        SAINTPLUS
_computing_data_reduction         SAINTPLUS
_computing_structure_solution     SHELXTL
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'

_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor
wR and
 goodness of fit S are based on F^2^, conventional R-factors R are
based
 on F, with F set to zero for negative F^2^. The threshold expression
of
```

```
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0801P)^2^+108.8290P] where P=(Fo^2^+2Fc^2
^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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 'Flack H D (1983), Acta Cryst. A39, 876-881'
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_refine_ls_number_parameters      351
_refine_ls_number_restraints      195
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_refine_ls_goodness_of_fit_ref    1.056
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 _atom_site_refinement_flags
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 _atom_site_disorder_group
C1 C 0.903(2) 0.144(2) 0.4950(13) 0.151(10) Uani 1 1 d DU . .
C2 C 0.870(3) 0.176(3) 0.4711(18) 0.179(15) Uani 1 1 d DU . .
H2A H 0.8999 0.2011 0.4509 0.268 Uiso 1 1 calc R . .
H2B H 0.8616 0.2066 0.4861 0.268 Uiso 1 1 calc R . .
H2C H 0.8270 0.1404 0.4613 0.268 Uiso 1 1 calc R . .
C3 C 0.964(3) 0.210(3) 0.5120(19) 0.220(18) Uani 1 1 d DU . .
H3A H 0.9897 0.1969 0.5282 0.330 Uiso 1 1 calc R . .
H3B H 0.9466 0.2341 0.5259 0.330 Uiso 1 1 calc R . .
H3C H 0.9931 0.2383 0.4925 0.330 Uiso 1 1 calc R . .
C4 C 0.862(4) 0.100(3) 0.5285(18) 0.24(2) Uani 1 1 d DU . .
H4A H 0.8885 0.0848 0.5418 0.358 Uiso 1 1 calc R . .
H4B H 0.8201 0.0613 0.5198 0.358 Uiso 1 1 calc R . .
H4C H 0.8508 0.1273 0.5447 0.358 Uiso 1 1 calc R . .
C5 C 0.852(2) 0.220(2) 0.2937(13) 0.123(10) Uani 1 1 d DU . .
H5A H 0.8068 0.1958 0.2831 0.147 Uiso 1 1 calc R . .
H5B H 0.8723 0.2679 0.2880 0.147 Uiso 1 1 calc R . .
```

```
C6 C 0.846(3) 0.211(4) 0.3361(13) 0.19(2) Uani 1 1 d DU . .
H6A H 0.8916 0.2348 0.3472 0.232 Uiso 1 1 calc R . .
H6B H 0.8257 0.1626 0.3424 0.232 Uiso 1 1 calc R . .
C7 C 0.801(4) 0.240(4) 0.352(2) 0.24(3) Uani 1 1 d DU . .
H7A H 0.8212 0.2879 0.3449 0.288 Uiso 1 1 calc R . .
H7B H 0.7557 0.2153 0.3411 0.288 Uiso 1 1 calc R . .
C8 C 0.795(4) 0.234(5) 0.395(2) 0.27(3) Uani 1 1 d DU . .
H8A H 0.7669 0.2526 0.4034 0.402 Uiso 1 1 calc R . .
H8B H 0.8396 0.2593 0.4058 0.402 Uiso 1 1 calc R . .
H8C H 0.7739 0.1868 0.4019 0.402 Uiso 1 1 calc R . .
C9 C 0.970(2) 0.237(3) 0.2911(15) 0.146(13) Uani 1 1 d U . .
H9A H 0.9701 0.2308 0.3178 0.175 Uiso 1 1 calc R . .
H9B H 0.9970 0.2189 0.2799 0.175 Uiso 1 1 calc R . .
C10 C 1.003(3) 0.309(3) 0.2833(18) 0.172(18) Uani 1 1 d U . .
H10A H 0.9803 0.3301 0.2967 0.206 Uiso 1 1 calc R . .
H10B H 1.0009 0.3171 0.2569 0.206 Uiso 1 1 calc R . .
C11 C 1.080(3) 0.342(4) 0.296(2) 0.20(2) Uani 1 1 d U . .
H11A H 1.1067 0.3315 0.2791 0.246 Uiso 1 1 calc R . .
H11B H 1.0830 0.3257 0.3210 0.246 Uiso 1 1 calc R . .
C12 C 1.104(4) 0.421(4) 0.296(3) 0.25(3) Uani 1 1 d U . .
H12A H 1.1510 0.4474 0.3034 0.382 Uiso 1 1 calc R . .
H12B H 1.0763 0.4295 0.3140 0.382 Uiso 1 1 calc R . .
H12C H 1.0975 0.4346 0.2721 0.382 Uiso 1 1 calc R . .
C13 C 0.891(3) 0.207(3) 0.2355(14) 0.140(13) Uani 1 1 d U . .
H13A H 0.9046 0.2551 0.2322 0.167 Uiso 1 1 calc R . .
H13B H 0.8435 0.1803 0.2273 0.167 Uiso 1 1 calc R . .
C14 C 0.935(4) 0.190(4) 0.2099(17) 0.20(2) Uani 1 1 d DU . .
H14A H 0.9196 0.1417 0.2113 0.238 Uiso 1 1 calc R . .
H14B H 0.9825 0.2149 0.2186 0.238 Uiso 1 1 calc R . .
C15 C 0.933(4) 0.210(4) 0.1688(16) 0.23(2) Uani 1 1 d DU . .
H15A H 0.8860 0.1888 0.1609 0.270 Uiso 1 1 calc R . .
H15B H 0.9529 0.2593 0.1673 0.270 Uiso 1 1 calc R . .
C16 C 0.972(4) 0.189(4) 0.141(2) 0.28(3) Uani 1 1 d DU . .
H16A H 0.9666 0.2007 0.1165 0.417 Uiso 1 1 calc R . .
H16B H 0.9542 0.1402 0.1430 0.417 Uiso 1 1 calc R . .
H16C H 1.0201 0.2123 0.1476 0.417 Uiso 1 1 calc R . .
C17 C 0.867(3) 0.119(3) 0.2833(17) 0.158(14) Uani 1 1 d U . .
H17A H 0.8766 0.1132 0.3088 0.190 Uiso 1 1 calc R . .
H17B H 0.8909 0.1036 0.2673 0.190 Uiso 1 1 calc R . .
C18 C 0.787(4) 0.072(3) 0.2764(19) 0.193(19) Uani 1 1 d DU . .
H18A H 0.7669 0.0375 0.2959 0.232 Uiso 1 1 calc R . .
H18B H 0.7648 0.0990 0.2762 0.232 Uiso 1 1 calc R . .
C19 C 0.780(4) 0.038(4) 0.239(2) 0.27(3) Uani 1 1 d DU . .
H19A H 0.8120 0.0210 0.2353 0.327 Uiso 1 1 calc R . .
H19B H 0.7824 0.0661 0.2179 0.327 Uiso 1 1 calc R . .
C20 C 0.706(4) -0.021(4) 0.247(3) 0.26(3) Uani 1 1 d DU . .
H20A H 0.6893 -0.0529 0.2273 0.392 Uiso 1 1 calc R . .
H20B H 0.6766 -0.0013 0.2505 0.392 Uiso 1 1 calc R . .
H20C H 0.7060 -0.0436 0.2699 0.392 Uiso 1 1 calc R . .
O1 O 1.0395(11) 0.2445(10) 0.3818(9) 0.087(6) Uani 1 1 d U . .
O2 O 0.9954(12) 0.1576(10) 0.4410(9) 0.081(4) Uani 1 1 d U . .
O3 O 0.9166(10) 0.1221(9) 0.3789(9) 0.071(4) Uani 1 1 d U . .
O4 O 0.7830(10) 0.0203(11) 0.3804(9) 0.090(5) Uani 1 1 d U . .
O5 O 0.8690(10) 0.0449(11) 0.4409(9) 0.083(4) Uani 1 1 d U . .
O6 O 0.8325(9) -0.0656(10) 0.3986(9) 0.071(4) Uani 1 1 d U . .
O7 O 0.9695(8) 0.0471(8) 0.3968(9) 0.060(3) Uani 1 1 d U . .
O8 O 0.8759(9) 0.0062(9) 0.3371(9) 0.063(3) Uani 1 1 d U . .
O9 O 0.8627(9) -0.1135(9) 0.3368(9) 0.063(4) Uani 1 1 d U . .
O10 O 1.0000 0.0000 0.3360(11) 0.060(4) Uani 1 3 d SU . .
O11 O 0.8393(11) -0.0683(11) 0.2707(9) 0.087(6) Uani 1 1 d U . .
O12 O 0.9535(9) -0.0795(10) 0.2816(9) 0.074(5) Uani 1 1 d U . .
O13 O 0.9612(14) 0.0545(16) 0.4920(10) 0.126(8) Uani 1 1 d U . .
Si1 Si 1.0000 0.0000 0.3846(8) 0.055(2) Uani 1 3 d SU . .
Si2 Si 0.9336(6) 0.0997(6) 0.4667(8) 0.109(3) Uani 1 1 d U . .
W1 W 1.01519(8) 0.16093(7) 0.3882(7) 0.0719(5) Uani 1 1 d U . .
W2 W 0.86092(7) 0.02683(7) 0.3870(7) 0.0727(5) Uani 1 1 d U . .
```

```
W3 W 0.90068(7) -0.04196(7) 0.3032(7) 0.0713(4) Uani 1 1 d U . .
N1 N 0.8932(18) 0.195(2) 0.2761(13) 0.143(9) Uani 1 1 d U . .
C2S C 1.0000 0.0000 0.1378(15) 1.2(9) Uiso 1 3 d SDU . .
C1S C 0.951(5) -0.020(7) 0.171(2) 0.7(7) Uiso 0.33 1 d PDU . .
N1S N 0.915(9) -0.037(10) 0.197(3) 0.27(10) Uiso 0.33 1 d PDU . .

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C2 0.20(3) 0.16(3) 0.21(3) -0.07(2) 0.01(2) 0.11(2)
C3 0.22(3) 0.19(3) 0.20(3) -0.10(2) -0.02(2) 0.068(19)
C4 0.25(4) 0.26(3) 0.20(3) 0.01(2) 0.11(3) 0.12(2)
C5 0.12(2) 0.12(3) 0.143(17) -0.01(2) -0.05(2) 0.07(2)
C6 0.16(5) 0.30(8) 0.16(2) 0.06(4) 0.01(4) 0.14(5)
C7 0.24(4) 0.25(4) 0.23(3) -0.02(3) 0.05(3) 0.13(3)
C8 0.28(5) 0.27(5) 0.23(3) -0.05(3) 0.03(3) 0.12(3)
C9 0.17(2) 0.21(2) 0.13(3) 0.03(3) -0.01(2) 0.147(19)
C10 0.16(3) 0.22(2) 0.18(5) 0.05(4) 0.00(3) 0.12(2)
C11 0.18(2) 0.25(3) 0.19(4) 0.01(3) -0.04(3) 0.11(2)
C12 0.24(4) 0.24(3) 0.25(4) 0.01(3) 0.00(3) 0.10(2)
C13 0.19(4) 0.15(4) 0.139(16) 0.02(2) -0.02(2) 0.13(3)
C14 0.24(7) 0.20(6) 0.20(3) 0.03(5) 0.05(5) 0.14(5)
C15 0.25(4) 0.24(4) 0.18(2) 0.00(3) 0.03(3) 0.12(3)
C16 0.29(5) 0.29(5) 0.24(3) -0.02(3) 0.08(3) 0.14(3)
C17 0.22(3) 0.180(19) 0.15(4) 0.04(2) -0.01(3) 0.158(19)
C18 0.23(4) 0.16(3) 0.23(5) 0.06(3) 0.00(4) 0.123(19)
C19 0.24(4) 0.28(4) 0.28(4) -0.03(3) -0.04(3) 0.12(3)
C20 0.26(4) 0.22(4) 0.30(4) 0.01(3) -0.03(3) 0.12(3)
O1 0.097(12) 0.057(7) 0.103(13) -0.015(8) 0.016(12) 0.036(8)
O2 0.090(10) 0.071(9) 0.087(8) -0.016(6) -0.007(7) 0.043(8)
O3 0.078(7) 0.066(6) 0.072(10) -0.005(7) 0.009(8) 0.038(6)
O4 0.070(7) 0.103(14) 0.103(13) 0.006(12) 0.018(8) 0.047(9)
O5 0.075(9) 0.094(11) 0.085(7) 0.003(7) 0.023(6) 0.047(8)
O6 0.049(9) 0.071(7) 0.075(11) 0.016(7) 0.012(9) 0.015(7)
O7 0.045(6) 0.051(6) 0.073(9) -0.003(7) 0.015(6) 0.016(6)
O8 0.056(9) 0.052(8) 0.074(7) 0.009(6) 0.004(6) 0.022(9)
O9 0.069(9) 0.062(8) 0.059(9) -0.006(7) -0.017(7) 0.033(7)
O10 0.062(7) 0.062(7) 0.055(9) 0.000 0.000 0.031(3)
O11 0.098(13) 0.112(16) 0.051(9) -0.001(8) -0.028(9) 0.051(12)
O12 0.072(11) 0.061(12) 0.075(11) -0.012(8) -0.002(7) 0.023(9)
O13 0.126(19) 0.18(2) 0.058(13) 0.036(13) 0.014(11) 0.063(17)
Si1 0.051(3) 0.051(3) 0.062(6) 0.000 0.000 0.0254(17)
Si2 0.110(8) 0.115(8) 0.094(6) -0.006(5) 0.002(4) 0.052(6)
W1 0.0745(9) 0.0573(9) 0.0877(11) -0.0034(7) 0.0019(8) 0.0358(7)
W2 0.0618(9) 0.0722(9) 0.0891(11) 0.0031(8) 0.0067(7) 0.0373(8)
W3 0.0658(9) 0.0764(10) 0.0691(8) -0.0007(7) -0.0078(7) 0.0337(8)
N1 0.123(16) 0.20(2) 0.166(18) 0.13(2) 0.050(17) 0.122(14)

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;
 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
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 treatment of cell esds is used for estimating esds involving l.s.
planes.
;

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 _geom_bond_atom_site_label_2
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 _geom_bond_site_symmetry_2
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C1 C4 1.54(2) . ?
C1 C3 1.55(2) . ?
C1 Si2 1.79(5) . ?
C2 H2A 0.9600 . ?
C2 H2B 0.9600 . ?
C2 H2C 0.9600 . ?
C3 H3A 0.9600 . ?
C3 H3B 0.9600 . ?
C3 H3C 0.9600 . ?
C4 H4A 0.9600 . ?
C4 H4B 0.9600 . ?
C4 H4C 0.9600 . ?
C5 N1 1.44(5) . ?
C5 C6 1.54(2) . ?
C5 H5A 0.9700 . ?
C5 H5B 0.9700 . ?
C6 C7 1.57(9) . ?
C6 H6A 0.9700 . ?
C6 H6B 0.9700 . ?
C7 C8 1.55(2) . ?
C7 H7A 0.9700 . ?
C7 H7B 0.9700 . ?
C8 H8A 0.9600 . ?
C8 H8B 0.9600 . ?
C8 H8C 0.9600 . ?
C9 C10 1.44(7) . ?
C9 N1 1.60(6) . ?
C9 H9A 0.9700 . ?
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C10 C11 1.58(7) . ?
C10 H10A 0.9700 . ?
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C11 C12 1.59(10) . ?
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C11 H11B 0.9700 . ?
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C12 H12B 0.9600 . ?
C12 H12C 0.9600 . ?
C13 N1 1.49(5) . ?
C13 C14 1.55(7) . ?
C13 H13A 0.9700 . ?
C13 H13B 0.9700 . ?
C14 C15 1.55(2) . ?
C14 H14A 0.9700 . ?
C14 H14B 0.9700 . ?
C15 C16 1.54(2) . ?
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C16 H16A 0.9600 . ?
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C16 H16C 0.9600 . ?
C17 N1 1.52(6) . ?
C17 C18 1.57(8) . ?
C17 H17A 0.9700 . ?
C17 H17B 0.9700 . ?
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O2 W1 1.94(2) . ?
O3 W2 1.890(18) . ?
O3 W1 1.966(19) . ?
O4 W2 1.70(2) . ?
O5 Si2 1.64(2) . ?
O5 W2 1.97(2) . ?
O6 W2 1.894(19) . ?
O6 W1 1.92(2) 2_645 ?
O7 Si1 1.586(17) . ?
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O7 W2 2.280(17) . ?
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O8 W2 1.925(18) . ?
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O9 W1 1.961(18) 2_645 ?
O10 Si1 1.75(3) . ?
O10 W3 2.275(15) . ?
O10 W3 2.275(15) 2_645 ?
O10 W3 2.275(15) 3_765 ?
O11 W3 1.679(18) . ?
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O12 W3 1.957(19) 2_645 ?
O13 Si2 1.70(3) . ?
Si1 O7 1.586(17) 2_645 ?
Si1 O7 1.586(17) 3_765 ?
W1 O6 1.92(2) 3_765 ?
W1 O9 1.961(18) 3_765 ?
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C1 C2 H2B 109.5 . . ?
H2A C2 H2B 109.5 . . ?
C1 C2 H2C 109.5 . . ?
H2A C2 H2C 109.5 . . ?
H2B C2 H2C 109.5 . . ?
C1 C3 H3A 109.5 . . ?
C1 C3 H3B 109.5 . . ?
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H3A C3 H3C 109.5 . . ?
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C1 C4 H4B 109.5 . . ?
H4A C4 H4B 109.5 . . ?
C1 C4 H4C 109.5 . . ?
H4A C4 H4C 109.5 . . ?
H4B C4 H4C 109.5 . . ?
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C6 C5 H5A 108.5 . . ?
N1 C5 H5B 108.5 . . ?
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H5A C5 H5B 107.5 . . ?
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C7 C6 H6A 109.7 . . ?
C5 C6 H6B 109.7 . . ?
C7 C6 H6B 109.7 . . ?
H6A C6 H6B 108.2 . . ?
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C8 C7 H7B 109.2 . . ?
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C7 C8 H8A 109.5 . . ?
C7 C8 H8B 109.5 . . ?
H8A C8 H8B 109.5 . . ?
C7 C8 H8C 109.5 . . ?
H8A C8 H8C 109.5 . . ?
H8B C8 H8C 109.5 . . ?
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N1 C9 H9A 108.9 . . ?
C10 C9 H9B 108.9 . . ?
N1 C9 H9B 108.9 . . ?
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C10 C11 H11B 111.6 . . ?
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H12A C12 H12C 109.5 . . ?
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C13 C14 C15 113(5) . . ?
C13 C14 H14A 109.1 . . ?
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C14 C15 H15B 108.6 . . ?
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C18 C17 H17B 108.7 . . ?
H17A C17 H17B 107.6 . . ?
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W2 O3 W1 116.0(9) . . ?
Si2 O5 W2 131.8(12) . . ?
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Si1 O7 W2 127.0(9) . . ?
W1 O7 W2 92.3(7) . . ?
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W3 O9 W1 149.6(10) . 2_645 ?
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Si1 O10 W3 121.3(6) . 2_645 ?
W3 O10 W3 95.5(8) . 2_645 ?
Si1 O10 W3 121.3(6) . 3_765 ?
W3 O10 W3 95.5(8) . 3_765 ?
W3 O10 W3 95.5(8) 2_645 3_765 ?
W3 O12 W3 119.9(10) . 2_645 ?
O7 Si1 O7 112.6(7) 2_645 . ?
O7 Si1 O7 112.6(7) 2_645 3_765 ?
O7 Si1 O7 112.6(7) . 3_765 ?
O7 Si1 O10 106.1(8) 2_645 . ?
O7 Si1 O10 106.1(8) . . ?
O7 Si1 O10 106.1(8) 3_765 . ?
O2 Si2 O5 111.1(13) . . ?
O2 Si2 O13 111.1(13) . . ?
O5 Si2 O13 107.6(14) . . ?
O2 Si2 C1 106.8(17) . . ?
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O1 W1 O2 96.7(9) . . ?
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O6 W1 O9 88.2(7) 3_765 3_765 ?
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O1 W1 O3 97.8(9) . . ?
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O4 W2 O6 99.7(9) . . ?
O3 W2 O6 161.8(8) . . ?
O4 W2 O8 98.5(9) . . ?
O3 W2 O8 91.9(8) . . ?
O6 W2 O8 86.7(8) . . ?
O4 W2 O5 98.0(9) . . ?
O3 W2 O5 88.7(9) . . ?
O6 W2 O5 87.4(9) . . ?
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O11 W3 O8 103.0(9) . . ?
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O8 W3 O10 86.4(7) . . ?
O12 W3 O10 72.5(7) . . ?
O12 W3 O10 72.1(7) 3_765 . ?
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C5 N1 C17 113(3) . . ?
C13 N1 C17 110(4) . . ?
C5 N1 C9 109(4) . . ?
C13 N1 C9 110(3) . . ?
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W3 O10 Si1 O7 178.1(6) 3_765 . . 2_645 ?
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W3 O10 Si1 O7 178.1(6) 2_645 . . . ?
W3 O10 Si1 O7 58.1(6) 3_765 . . . ?
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Si1 O7 W1 O3 139.9(15) . . . . ?
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W1 O6 W2 O8 28(2) 2_645 . . . ?
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Si2 O5 W2 O8 54(4) . . . . ?
Si2 O5 W2 O7 38.0(16) . . . . ?
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C6 C5 N1 C17 58(6) . . . . ?
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C14 C13 N1 C17 -62(6) . . . . ?
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